Protein Crystallography Station (PCS)

The Bioscience Division has built a Protein Crystallography Station (PCS) at the LANSCE Manuel Lujan Jr. Neutron Scattering Center for the national structural biology community to investigate the structure and dynamics of proteins, biological polymers, and membranes. Emerging structural genomics efforts to solve the three-dimensional structures of thousands of proteins sequenced in genome projects are largely based on the use of synchrotron x-rays. However, certain unique types of information relating to structurally and functionally important water molecules and hydrogen atoms can only be obtained using neutrons. Despite the potential importance of neutrons, the number of studies so far has been limited by issues of access to neutron sources and appropriate instrumentation. In particular, the neutron flux and detector technologies on presently available instruments have led to prohibitively large sample size requirements. Large crystals of proteins are difficult to grow. The PCS, funded by the Department of Energy Office of Biological and Environmental Research, is the only resource of its kind in North America and the first to be built at a spallation neutron source. A number of technological innovations have been incorporated, including a partially coupled water moderator and a large cylindrical detector that, along with the improved LANSCE neutron source, will make data collection from smaller crystals feasible. These innovations will greatly broaden the application of neutrons to structural biology and make the PCS a benchmark for similar projects worldwide. Around twenty experiments will be accommodated each year during an eight-month run cycle.

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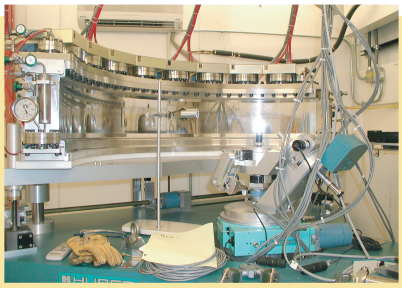
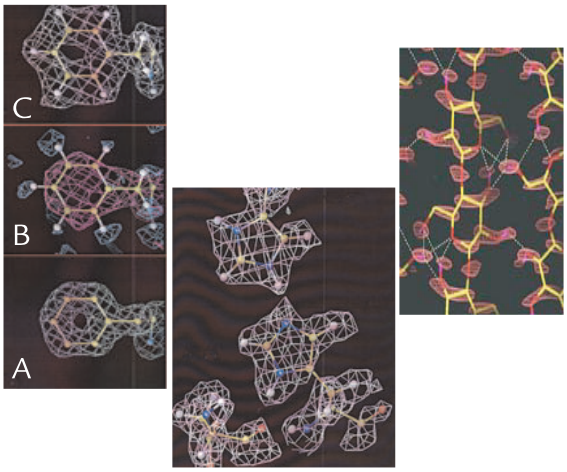


The PCS cylindrical neutron detector. The detector consists of an electrode structure contained in an aluminum pressure vessel. The pressure vessel is filled with a mixture of ^{3}He and propane. The ^{3}He has an extremely high cross section for thermal neutron absorption. Neutrons diffracted by the sample are absorbed by the ^{3}He. This interaction results in the creation of a proton and triton. These primary ionization products drift toward the nearest electrode-anode wire where they multiply in the high electric field near the wire surface. The charges induced over different electrodes allow for the spatial detection of an event.

Details from the structure of myoglobin

Left and center details from the structure of myoglobin. Left (a), scattering density calculated from 1.8-Å x-ray data. Only C atoms are covered. Left (b), negative (blue) and positive (red) scattering density calculated from 2-Å neutron data. H with its strong negative scattering length is covered. Left (c), positive scattering density calculated from predeuterated myoglobin. Deuterium (D) with its strong positive scattering density is covered. Neutron diffraction can be used to locate H or D with data extending to less than 2-Å. Center, details of the 2.2-Å neutron map clearly reveal D positions. Right, neutron diffraction from fibers of biological polymers such as DNA and polysaccharides can reveal details of hydrogen bonding patterns and hydration.



Protein Crystallography Specifications	
Unit cell size	150 Å
Sample size	1 mm
d-spacing	1 Å–250 Å
Wavelength shaping	T_0 and T_1 choppers and tail-cutter
Wavelength range	1 Å–5 Å
Sample-to-detector distance	700 mm
Beam size	5 mm on detector
Resolution	1.2 mm
Detector area	2930 cm^2
Counting rate	> 1,000,000 c/s